FILE 'HOME' ENTERED AT 11:08:38 ON 18 APR 2005

=> file reg

=>

Uploading C:\Program Files\Stnexp\Queries\10087756.str

chain nodes : 11 12 13 14 15 16 23 24 31 32 33 34 35 36 37 38 ring nodes : 1 2 3 4 5 6 7 8 9 10 17 18 19 20 21 22 25 26 27 28 29 30 chain bonds : 2-25 3-11 7-12 8-13 10-17 13-14 13-15 15-16 18-23 20-24 27-32 28-31 30-33 30-38 33-34 33-37 34-35 34-36 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 17-18 17-22 18-19 19-20 20-21 21-22 25-26 25-29 26-27 27-28 27-30 28-29 28-30 exact/norm bonds : 2-25 5-7 6-10 7-8 7-12 8-9 9-10 10-17 13-14 13-15 15-16 25-26 25-29 26-27 27-28 27-30 28-29 28-30 30-33 33-34 34-35 exact bonds : 3-11 8-13 18-23 20-24 27-32 28-31 30-38 33-37 34-36 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS

Ll STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

STR

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full 3 SEA SSS FUL L1

=> file ca

=> s 14 L5 3 L4

=> d ibib abs fhitstr hitrn 1-3

L5 ANSWER 1 OF 3 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 134:147591 CA
FITLE: Preparation of trovafloxacin
Chiu, Charles K., Wint, Levin T.
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: U.S., 7 pp.
CODEN: USXXAM

DOCUMENT TYPE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND DX	75	API	PLICATION NO.		DATE
		010206		1999-236737	-	19990125
US 6184380 US 2002095043		020718		2002-87756		20020304
PRIORITY APPLN. INFO.:	(US	1998-71601P	P	19980116
				1999-236737		19990125
	-			2000-718324		20001122

The title process comprises use of azabicyclohexanes I [R1 = (un)substituted CH2Ph: R2 = CF3, alkyl, (un)substituted Ph) and a 7-chloro-6-fluoro-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylic acid alkyl ester.
323575-31-1P
RE: IMF (Industrial manufacture): RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation of trovafloxacin)
323575-31-1 CA
1,8-Naphthyridine-3-carboxylic acid, 7-[6-(acetylamino)-3-azabicyclo[3.1.0]hex-3-yl]-1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-4-oxo-, ethyl ester (SCI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 131:116223 CA
TITLE: Process for preparing naphthyridones and intermediates
INVENTOR(s): Chiu, Charles Kwok-Fung, Wint, Lewin Theophilus
FAIENT ASSIGNEE(s): SOURCE: Chiu, Charles Kwok-Fung, Wint, Lewin Theophilus
FAIENT TYPE.

DOCUMENT TYPE:

English 2 FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
EP 930297	A1 (19990721)	EP 1999-300183	19990112
EP 930297	B1 20030423	2	
		, GR, IT, LI, LU, NL,	SE. MC. PT.
	LV, FI, RO	,,,,,	,,
AU 9897115	A1 19990805	AU 1998-97115	19981215
JP 11255745	A2 19990921	JP 1999-5494	19990112
SG 76584	A1 20001121	SG 1999-46	19990112
EG 21514	A 20011128	EG 1999-34	19990112
TW 483890	B 20020421	TW 1999-88100415	19990112
AT 238281	E 20030515	AT 1999-300183	19990112
PT 930297	T 20030829	PT 1999-300183	19990112
ES 2195513	T3 20031201	ES 1999-300183	19990112
BR 9900066	A 20000509	BR 1999-66	19990114
CA 2258960	C 20020903	CA 1999-2258960	19990114
CA 2258960	AA 19990716		
NO 9900185	A 19990719	NO 1999-185	19990115
CN 1228422	A 19990915	CN 1999-101086	19990115
NZ 333769	A 20000327	NZ 1999-333769	19990115
ZA 9900277	A 20000717	ZA 1999-277	19990115
BG 64094	B1 20031231	BG 1999-103087	19990115
PRIORITY APPLN. INFO.:		US 1998-71601P	P 19980116
OTHER SOURCE(S): GI	CASREACT 131:11622	3; MARPAT 131:116223	

	F CO2R3	
R ² CHN H	C1 N N	
H NR1	F 11	

6-Acetamido-3-benzylazabicyclo[3.1.0]hemanes [I; Rl = (un)substituted PhCH2; R2 = Cl-6 alkyl, CF3, (un)substituted Ph] are prepared by reduction

the parent nitro derivs. with Fe powder in AcCH/Me2CHUH and N-acylation of the resulting anines. Debenzylation of I with H in AcCH in the presence of Pd catalyst, condensation of debenzylated intermediates with naphthyridine-3-carboxylate esters (II: N3 = C1-6 alkyl) and hydrolysis of

L5 ANSWER 1 OF 3 CA COPYRIGHT 2005 ACS on STN (Continued)

ΙT 323575-31-1P

RI: IMP (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of trowsflowsoin)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 3 CA COPYRIGHT 2005 ACS on STN (Continued) the resulting intermediates (preps. procedure claimed) with MeSO3H in aq. org. solvents gives trovafloxacin (III), an antibacterial active esp. against gram-pos. bacterial strains, as monomethanesulfonate salt. Thus, III-HO3SMe was prepd. from I (R1 - PhCH2, R2 - Me) and II (R3 - Et) as described above.
222598-25-3P

232598-25-39
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis with methanesulfonic acid; process for

aring
naphthyridones and trovafloxacin intermediates)
232598-25-3 CA
1,8-Naphthyridine-3-carboxylic acid, 7-[(1α,5α,6α)-6(acetylamino)-3-azabicyclo[3.1.0]hex-3-yl]-1-(2,4-difluorophenyl)-6-fluoro1,4-dihydro-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

232598-25-3P

232598-23-39
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
[preparation and hydrolysis with methanesulfonic acid; process for

preparing
naphthyridones and trovafloxacin intermediates)
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 3 CA ACCESSION NUMBER: TITLE:

CCPYRIGHT 2005 ACS on STN
126:157823 CA
Process for preparing szabicyclo naphthyridine
carbcrylic acid dipeptide prodrug
Braish, Tamin F., Castaldi, Hichael J., Vatson, Harry
A., Jr.
Pfizer Inc., USA, Braish, Tamin F., Castaldi, Hichael
J., Vatson, Harry A., Jr.
PCT Int. Appl., 26 pp.
CUDEN: PIXXO2
Patent
English
1 PATENT ASSIGNER(S):

SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAIENT NO. KIND DATE APPLICATION NO. DATE	PAIRAL INFORMATION:			
WO 9700268				
W: CA, JP, NX, US SE PKY AT, BE, CH, DE, DX, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE CA 2224616 AA 19970103 CA 1996-2224616 19960327 CA 2224616 C 20000502 EP 1996-904996 19960327 EF 833837 A1 1998003E EP 1996-904996 19960327 EF 833837 A1 1998013T ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI JF 3029293 B2 20000404 JP 1997-502832 19960327 JP 10511983 T2 19981117 1996-904996 19960327 19960327 AT 221544 E 20020129 PT 1996-904996 19960327 19960327 ES 2178701 T3 20030101 ES 1996-904996 19960327 19960327 US 5393550 A 19990817 US 1998-981350 19980311 PRIORITY APPLIN. INFO: WO 1996-18257 W 19960327 OTHER SOURCE(S): MARPAT 126:157823 MAPPAT 126:157823 WO 1996-18257 W 19960327				
W: AT, EE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, NC, NL, PT, SE CA 2224616	WO 9700268	A1 19970103	WO 1996-IB257	19960327
CA 2224616 AA 19970103 CA 1996-2224616 19960327 CA 22224616 C C 20000502 EP 833837 A1 19980408 EP 1996-904996 19960327 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, L1, LU, NL, SE, PT, IE, FI JF 30329293 B2 20000404 JP 1997-502832 19960327 JF 10511983 T2 19981117 AT 221544 E 200220915 AT 1996-904996 19960327 FF 233337 T 20021129 PT 1996-904996 19960327 ES 2178701 T3 20031010 ES 1996-904996 19960327 US 5939550 A 19990817 US 1998-981350 19980311 PRIORITY APPLIN. INFO:: US 1998-981350 19980311 PRIORITY APPLIN. INFO:: US 1998-190827 A1 19950155 OTHER SOURCE(S): MARPAT 126:157823	₩: CA, JP, MX,	us		
CA 2224616 AA 19970103 CA 1996-2224616 19960327 CA 22224616 C C 20000502 EP 833837 A1 19980408 EP 1996-904996 19960327 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, L1, LU, NL, SE, PT, IE, FI JF 30329293 B2 20000404 JP 1997-502832 19960327 JF 10511983 T2 19981117 AT 221544 E 200220915 AT 1996-904996 19960327 FF 233337 T 20021129 PT 1996-904996 19960327 ES 2178701 T3 20031010 ES 1996-904996 19960327 US 5939550 A 19990817 US 1998-981350 19980311 PRIORITY APPLIN. INFO:: US 1998-981350 19980311 PRIORITY APPLIN. INFO:: US 1998-190827 A1 19950155 OTHER SOURCE(S): MARPAT 126:157823	RV: AT, BE, CH,	DE, DK, ES, FI.	FR. GB. GR. IE. IT. I	U, MC, NL, PT, SE
CA 2224616 C 20000502 EP 833837 A1 19980408 EP 1996-904996 19960327 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI JP 3029293 B2 20000404 JP 1997-502832 19960327 AT 221544 E 20020815 AT 1996-904996 19960327 PT 833837 T 20021129 PT 1996-904996 19960327 ES 2178701 T3 20031010 ES 1996-904996 19960327 US 5939550 A 19990817 US 1998-981350 19980317 PRIORITY APPIM. INFO:: OTHER SOURCE(S): MARPAT 126:157823				
EF 833837 A1 19980408 EP 1996-904996 19960327 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI JF 3029293 B2 20000404 JP 1997-502832 19960327 AT 221544 E 200220815 AT 1996-904996 19960327 FF 133837 T 20021129 PT 1996-904996 19960327 ES 2178701 T3 20031010 ES 1996-904996 19960327 US 5939550 A 19990817 US 1998-981350 19960327 PRIORITY APPLN. INFO:: US 1998-981350 19980311 PRIORITY APPLN. INFO:: US 1998-190827 W 19960327 OTHER SOURCE(S): MARPAT 126:157823				
FF 933937 B1 20020731 R: AT, EE, C, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI JP 3029293 B2 20000404 JP 1997-502932 19960327 AT 221544 E 20020915 AT 1996-904996 19960327 FF 833837 T 20021129 PT 1996-904996 19960327 ES 2178701 T3 20031010 ES 1996-904996 19960327 US 5939550 A 19990817 US 1998-991350 19980317 PRIORITY APPLM. INFO:: US 1995-90827 A 19950615 OTHER SOURCE(S): MARPAT 126:157823	EP 833837	A1 19980408	EP 1996-904996	19960327
R: AT, BE, CH, DE, DK, RS, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI JP 302293 B2 2000404 JP 1997-502832 19960327 JP 10511983 T2 19981117 AT 221544 E 20022015 A1 1996-904996 19960327 ES 2178701 T3 2003101 ES 1996-904996 19960327 US 5393550 A 19990817 US 1996-904996 19960327 PRIORITY APPLN. INFO:: US 1998-91350 19980321 PRIORITY APPLN. INFO:: US 1998-91350 19980311 OTHER SOURCE(S): MARPAT 126:157823				
JF 3029293 B2 20000404 PP 1997-502832 19960327 JP 10511993 T2 19981117 FP 1998117 FP 1998117 FP 1998117 FP 1998117 FP 1998175 FP 199				II. SR. PT. IR. FI
JP 10511993 T2 1998117 AT 221544 E 20020815 AT 1996-904996 19960327 PT 833837 T 200201129 PT 1996-904996 19960327 ES 2178701 T3 20030101 ES 1996-904996 19960327 US 5939550 A 19990817 US 1998-91350 19980311 PRIORITY APPLN. INFO:: US 1998-91350 19980311 OTHER SOURCE(S): MARPAT 126:157823				
AT 221544 E 20020915 AT 1996-904996 19960327 PT 91896-904996 19960327 PT 91896-904996 19960327 PT 1996-904996 19960327 PT 1996-904996 19960327 PT 1996-904996 19960327 PT 1996-904996 19960327 PT 1996				13300327
US 5939550 A 19990817 US 1998-981350 19980311 PRIORITY APPIM. INFO.: US 1995-690827 A1 19950615 VD 1996-1B257 V 19960327 OTHER SOURCE(S): MARPAT 126:157823	NT 221544	P 20020016	3T 1006.004006	10060337
US 5939550 A 19990817 US 1998-981350 19980311 PRIORITY APPIM. INFO.: US 1995-690827 A1 19950615 VD 1996-1B257 V 19960327 OTHER SOURCE(S): MARPAT 126:157823	NI 221344	20020813	AT 1990-904990	19900327
US 5939550 A 19990817 US 1998-981350 19980311 PRIORITY APPIM. INFO.: US 1995-690827 A1 19950615 VD 1996-1B257 V 19960327 OTHER SOURCE(S): MARPAT 126:157823	P1 833837	20021129	PI 1996-904996	19960327
PRIORITY APPLN. INFO.: US 1995-490827 A1 19950615 W 1996-1B257 OTHER SOURCE(S): HARPAT 126:157823	ES 21/8/01	T3 20030101	ES 1996-904996	19960327
WO 1996-IB257 W 19960327 OTHER SOURCE(S): MARPAT 126:157823		A 19990817		
OTHER SOURCE(S): MARPAT 126:157923	PRIORITY APPLN. INFO.:			
			WO 1996-IB257	W 19960327
	OTHER SOURCE(S):	MARPAT 126:1578	23	
GI .	GI			

A process is given for preparing a pharmaceutically acceptable acid addition salt of prodrug acid I. Thus, N-Boc protected 7-{{1 α , 5 α , 6 α }-6-amino-3-azabicycle{3.1.0}hex-3-y1]-6-fluoro-1-{2,4}-difluorophenyl-1,4-dihydro-4-axo-1,8-naphthyridine-3-carboxylic acid Et ester, Boc-Q-OEt, (Boc = tert-butoxycarbonyl) was deprotected by

- ANSWER 3 OF 3 CA COPYRIGHT 2005 ACS on STN (Continued) trifluoroacetic acid and the product coupled with Boc-Ala-Ala-OH using EEDQ and then treated with rethanesulfonic acid to afford I resylate. The latter prodrug serves as a water-sol. prodrug companion to known antibacterial agent H-Q-CH. its 1712-86-1P
 RL: RCT (Reactant), SPN (Synthetic preparation), FREP (Preparation), RACT (Reactant or reagent) (prepn.of arabicyclo naphthyridine carboxylic acid dipeptide prodrug) 186772-86-1 CA
 L-Alaninamide, N-[{1,1-dimethylethoxy)carbonyl}-L-alanyl-N-[(16,50,60)-3-[8-(2,4-difluorophenyl)-6-(ethoxycarbonyl)-3-azabicyclo[3.1.0]hex-6-y1]- (CA INDEX NAME)

Absolute stereochemistry.

186772-86-1P
RL: RCT (Reactant), SPN (Synthetic preparation), PREP (Preparation), RACT (Reactant or reagent)
(prepn.of azabicyclo naphthyridine carboxylic acid dipeptide prodrug)

=> file casreact

=> s l1 full

FULL SEARCH INITIATED 11:10:33 FILE 'CASREACT'

SCREENING COMPLETE - 121 REACTIONS TO VERIFY FROM 6 DOCUMENTS

2 DOCS

100.0% DONE 121 VERIFIED 10 HIT RXNS SEARCH TIME: 00.00.01

2 SEA SSS FUL L1 (10 REACTIONS)

=> d ibib abs rx

L7 ANSWER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 134:147591 CASREACT
TITLE: Preparation of trovafloxacia
Chiu, Charles K., Vint, Levin T.
PATENT ASSIGNEE(S): Pfizer Inc., USA
U.S., 7 pp.
CODEN: USXXXM
PATENT LANGUAGE: Patent
LANGUAGE: Regists
PATENT INFORMATION:

PATENT INFORMATION:

PATENT NO. KIND PATE APPLICATION NO. DATE

US 6184380 #1 20010206 US 1999-236737 19990125
US 2002095043 1 200020718 US 2002-87756 20020304
PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 34:147591

H
R2

NARPAT 34:147591

AB The title process comprises use of azabicyclohexanes I [R1 = (un)substituted CH2Ph; R2 = CF3, alkyl, (un)substituted Ph] and a 7-chloro-6-fluoro-1,4-dihydro-4-cxo-1,8-naphthyridine-3-carboxylic acid alkyl ester.

RX(3) OF 14 ...J + M ===> H...

L7 ANSWER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RX(4) RCT N 323575-31-1 RGT R 75-75-2 MeSO3H PRO Q 323575-32-2 SOL 71-36-3 BuOH, 7732-18-5 Water

RX(5) OF 14 ...# ===> T

L7 ANSVER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

N YIELD 95%

RX(3) RCT J 323575-30-0, M 100491-29-0

STAGE(1)
RGT 0 121-44-8 Et3N
SOL 141-78-6 Accet

STAGE(2)
SOL 7732-18-5 Water
PRO N 323575-31-1

RX(4) OF 14 ...# ---> Q

L7 ANSWER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

T: CM 2 YIELD 96%

RX(5) RCT N 323575-31-1 RGT R 75-75-2 MeSO3H PRO T 323575-34-4 SOL 64-17-5 EtOH

RX(7) OF 14 COMPOSED OF RX(2), RX(3) RX(7) C + E + M ===> #

STEPS

L7 ANSWER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

N YIELD 95%

RCT C 323575-28-6, E 64-19-7 RGT K 1333-74-0 H2 PRO J 323575-30-0 CAT 7440-05-3 Pd SOL 7732-18-5 Water RX (2)

RX (3) RCT J 323575-30-0, M 100491-29-0

STAGE(1) RGT O 121-44-8 Et3N SOL 141-78-6 Accet STAGE(2) SOL 7732-18-5 Water PRO N 323575-31-1

PX(10) OF 14 COMPOSED OF RX(1), RX(2), RX(3) PX(10) A + B + E + M ===> #

ANSWER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN RGT K 1333-74-0 H2 PRO J 323575-30-0 CAT 7440-05-3 Pd SOL 7732-18-5 Water RCT J 323575-30-0, M 100491-29-0 RX (3) STAGE(1) RGT O 121-44-8 Et3N SOL 141-78-6 AcOEt

STAGE(2)
SOL 7732-18-5 Water
PRO N 323575-31-1
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

(Continued)

L7 ANSWER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

N YIELD 95%

RX (1) RCT A 323575-35-5 STAGE(1) RGT D 7439-89-6 Fe, E 64-19-7 ACOH SOL 67-63-0 Me2CHOH

STAGE (2) RCT B 108-24-7

STAGE (3) RGT F 1310-73-2 NaOH SOL 7732-18-5 Vater, 75-09-2 CH2C12 PRO C 323575-28-6

RX (2) RCT C 323575-28-6, E 64-19-7

=> d ibib abs rx 2

L? ANSWER 2 OF 2
ACCESSION NUMBER:
131:116223 CASREACT
11TLE:
1IVENIOR(S):
PATENT ASSIGNEE(S):
SOURCE:
COURSEN TYPE:
LANGUAGE:
LANGUAGE:
AND ACC. NUM. COUNT:
2
CARREACT COPYRIGHT 2005 ACS on STN
131:116223 CASREACT
Process for presparing naphthyridones and intermediates
Chiu, Charles Xvok-Pung; Vint, Lewin Theophilus
Pfizer Products Inc., USA
COURSEN: EPXXUW

Patent
LANGUAGE:
Regist
R

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.

EP 930297
EP 930297
EP 930297
R: AT, BE, CH, DE, DE, SE, ST, LT, LV, FI, RO

AU 9897115
SG 76584
A1 29997021
EG 21514
A2 20001121
EG 21514
A2 20001121
EG 21514
A2 20001121
FF 930297
T 2030829
ES 2195513
T3 20031201
FF 930297
CA 2258960
CA 2000509
CA 258960
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CA 258960
CA 258960
CA 2000509
CA 258 PATENT NO. KIND DATE APPLICATION NO. DATE EP 1999-300183 19990112 GB, GR, IT, LI, LU, NL, SE, MC, PT, AU 1998-97115 19981215
JP 1999-5494 19990112
SG 1999-46 19990112
TV 1999-88100415 19990112
TV 1999-300183 19990112
PT 1999-300183 19990112
ES 1999-300183 19990114
CA 1999-258960 19990114 NO 1999-185 CN 1999-101086 NZ 1999-333769 ZA 1999-277 BG 1999-103087 US 1998-71601P 19990115 19990115 19990115 19990115 19990115 19980116 MARPAT 131:116223

6-Acetamido-3-benzylazabicyclo[3.1.0]hexanes [I; R1 = (un)substituted

ANSWER 2 OF 2 CASREACT COPYRIGHT 2005 ACS on STN PRO H 232598-23-1 SOL 64-17-5 EtOH (Continued)

RX(4) OF 14 ...R + B ===> G...

(4)

G YIELD 95%

RX (4) RCT R 100491-29-0, B 232613-59-1 STAGE(1) RGT S 121-44-8 Et3N SOL 141-78-6 AccEt STAGE(2) RGT P 7732-18-5 Water PRO G 232598-25-3

ANSWER 2 OF 2 -CASREACT COPYRIGHT 2005 ACS on STN (Continued)
PhCH2; R2 = C1-6 alkyl, CF3, (un) substituted Ph) are prepd. by redn. of
the parent nitro derivs. with Fe powder in AcOH/Me2CHOH and M-acylation of
the resulting anines. Debensylation of I with H in AcOH in the presence
of Pd catalyst, condensation of debensylated intermediates with
naphthyridines-3-carboxylate esters (II; R3 = C1-6 slkyl) and hydrolysis of
the resulting intermediates (prepn. procedure claimed) with MeSOHH in acorg. solvents gives trovaflowacin (III), an antibacterial active esp.
against gran-pos. bacterial strains, as monomethanesulfonate salt. Thus,
III:HO36Me was prepd. from I (R1 = PhCH2, R2 = Me) and II (R3 = Et)
as described above.

...G ===> H RX (2) OF 14

H: CM 2 YIELD 96%

RX (2) RCT G 232598-25-3 RGT I 75-75-2 MeSO3H

L7 ANSWER 2 OF 2 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RX(5) OF 14 ...G ===> U

U: CM 2 YIKLD 874

RCT G 232398-25-3 RGT I 75-75-2 MeSO3H PRO U 147059-75-4 SOL 7732-18-5 Water, 71-36-3 BuOH NTE extensive work-up to change crystal properties RX (5)

RX(6) OF 14 COMPOSED OF RX(1), RX(4) RX(6) A + R \Longrightarrow O

17 ANSWER 2 OF 2 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

G YIELD 95%

RX(1) RCT A 232598-24-2

STAGE(1)
RGT C 64-19-7 AcoH
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

STAGE(2)
RGT D 1333-74-0 H2
PRO B 232613-59-1

RX(4) RCT R 100491-29-0, B 232613-59-1

STAGE(1)
RGT S 121-44-8 Et3N

L7 ANSWER 2 OF 2 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

```
FX(3) RCT X 13021-02-8

STAGE(1)
RCT M 7439-89-6 Fe, C 64-19-7 ACOH
SOL 67-63-0 Me2CHOH

STAGE(2)
RCT L 108-24-7

STAGE(3)
SOL 67-63-0 Me2CHOH

STAGE(4)
RCT N 1310-73-2 NaOH
SOL 7732-18-5 Water, 107-06-2 C1CH2CH2C1

PRO A 232598-24-2

FX(1) RCT A 232598-24-2

STAGE(1)
RCT C 64-19-7 ACOH
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

STAGE(2)
RCT D 1333-74-0 H2
PRO B 232613-59-1

FX(4) RCT R 100491-29-0, B 232613-59-1

STAGE(1)
RCT S 121-44-8 Et3N
SOL 141-78-6 ACOET

STAGE(2)
RCT P 7732-18-5 Water
PRO G 232598-28-3

REFERENCE COUNT: 6
THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
```

L7 ANSWER 2 OF 2 CASREACT COPYRIGHT 2005 ACS on STN (Continued) SOL 141-78-6 ACCET

STAGE(2) RGT P 7732-18-5 Water PRO G 232598-25-3

RX(14) OF 14 COMPOSED OF RX(3), RX(1), RX(4) RX(14) K + L + R \Longrightarrow G

G YIELD 95%

=>

Uploading C:\Program Files\Stnexp\Queries\11087756.str

L8 STRUCTURE UPLOADED

=> d 18 L8 HAS NO ANSWERS

L8 STR

L9 ANSWER 1 OF 5 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 134:147591 CASREACT
ITITLE: Preparation of trovafloxacin
Chiu, Charles K.; Wint, Lewin T.
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: USXCAM DOCUMENT TYPE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. DATE APPLICATION NO. DATE 20010206 20020718 US 1999-236737 US 2002-87756 US 1998-71601P US 1999-236737 US 6184380 US 2002095043 B1 A1 19990125 20020304 19980116 PRIORITY APPLN. INFO.: OTHER SOURCE(S): MARRAT 134:147591

The title process comprises use of azabicyclohexanes I [R1 = (un)substituted CH2Ph: R2 = CF3, alkyl, (un)substituted Ph) and a 7-chloro-6-fluoro-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylic acid alkyl ester.

RX (4) OF 14 ...N ---> Q

L9 ANSWER 2 OF 5 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 133:222629 CASREACT
TITLE: Synthesis of trovafloxacin using various (1c, 5c, 6a)-3-azabicyclo[3.1.0]hexane derivatives derivatives
Norris, Timothy: Braish, Tamim F.; Butters, Michael;
DeVries, Keith M.; Hawkins, Joel M.; Massett, Stephen
S.; Rose, Peter R.; Santafianos, Dinos; Sklavounos,
Constantiar
Pfizer Central desearch Laboratories, Groton, CT,
06340, U8A
Perkin (2000) (10), 1615-1622
CODEN: EERFS
Royal Scriety of Chemistry
Journal
English AUTHOR(S): CORPORATE SOURCE: SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Trovafloxacin, a novel broad spectrum antibacterial, contains the unusual (1e, 5e, 6e)-3-azabicyclo(3.1.0) hexane ring system. The prototype of the industrial synthesis of this ring system and possible mechanistic pathways to exclusive formation of the exo or 6a-nitro derivative I are described, which leads to the key 6a-nitro-3-azabicyclo(3.1.0) hexane intermediate [II, R = NOZ, R 2 = Bn [III]). The synthesis of II (R1 = NNIZ, R2 = H) and useful protected exo 6-anino deriva. II (R1 = BOCR, PECH:N, R2 = H) follows from III. These can be coupled with the 7-chloronaphthyridone to yield protected trovafloxacin compds. IV [R3 = BOCR], NNIZ, PECH:N) in good yield. Removal of protecting groups from IV with methanesulfonic acid yields trovafloxacin mesylate from which the trovafloxacin reviterion can be liberated with hase treatment. The switterion can also be prepared directly from the tosylate salt of II (R1 = NNIZ, R2 = H) and naphthyridone-2-carboxylic acid V.

RX(16) OF 68 ...AM ---> AS...

L9 ANSWER 1 OF 5 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

Q: CM 2

N 323575-31-1

R 75-75-2 Meso3H

R 0 323575-32-2

71-36-3 BUOM, 7732-18-5 Water

NT:

9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT RX (4) REFERENCE

ANSWER 2 OF 5 CASREACT COPYRIGHT 2005 ACS on STN (Continued) AS: CM 1 YIELD 90%

RCT AM 134575-66-9 RGT AT 75-75-2 MeSO3H PRO AS 147059-75-4 SOL 109-99-9 THF COUNT: 13 TH RX (16)

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT REFERENCE COUNT:

L9 ANSWER 3 OF 5
ACCESSION NUMBER: 132:122609 CASREACT
ITILE: 132:122609 CASREACT
ITILE: Preparation of trovafloxacin and analogs
NORTH, TICOTHY
PATENT ASSIGNEE(S): Pfizer Products Inc., USA
BULP PATENT, 16 Fp.
CODEN: EFEXCES DOCUMENT TYPE: Patent English 1 FAMILY ACC. NUM. COUNT: PATENT INFORMATION: KIND DATE PATENT NO. APPLICATION NO. DATE PATEIT NO.

EF 976749

R: AT, BE, CH, DK, DK, ES, FR, GB, GR, IT, LI, LV, IE, SI, LT, LV, FI, RO
US 6114531

A 20000202

BF 1999-305577

IE, SI, LT, LV, FI, RO
US 6114531

A 20000202

JP 1999-324385

IP 2000053646

A2 20000222

JP 1999-3210179

CA 2278845

AA 20000128

AU 9941169

AI 20000217

AU 1999-41169

KR 2000012002

A 20000225

KR 1999-30560

JR 1990-3030

CH 1247865

A 20000322

CH 1999-19527

JR 1999-4814

AU 2010129

AU 1999-4814

AU 20000221

AU 1999-991796

AU 20000221

AU 1999-991796

AU 20000221

AU 1999-991796

AU 20000221

AU 1999-991796

AU 20000221

AU 1999-991796 20000202 19990714 NL, SE, MC, PT, US 6114531
JP 2000053646
CA 2278845
CA 2278845
AU 9941169
KR 2000012002
ER 9903003
CN 1247865
2A 9904814
RU 2167867
TR 9901796
PRIORITY APPLN. INFO.:
OTHER SOURCE(6): 19990602 JP 1999-210179 19990726 CA 1999-2278845 19990726 AU 1999-41169 KR 1999-30560 ER 1999-3003 CN 1999-119527 ZA 1999-4814 RU 1999-116268 TR 1999-9901796 MX 1999-7034 US 1998-94440P 19990727 19990727 19990727 19990727 19990727 OTHER SOURCE(S): MARPAT 132:122609

AB Title compds. [I; R = H2N(CH2)n21; R1 = Et, CMe3, cyclopropyl, etc.; R2 = H, F, alkyl, alkoxy, etc.; Z = CH, CF, CR3, N, etc.; R1R3 = atoms to complete a ring; Z1 = 1-aze (bi)cycloalkylene; n = 0 or 1] were prepared by condensation of I (R = halo) with an acid salt of H2N(CH2)n21H.

RX(6) OF 36 ...U + S ===> V

L9 ANSWER 3 OF 5 CASREACT COPYRIGHT 2005 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 5 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

(6)

YIELD 75%

RX(6) RCT U 100492-04-4, S 256369-34-3

STAGE(1) RGT W 121-44-8 Et3N SOL 67-56-1 MeOH

STAGE (2)
SOL 109-99-9 THF
PRO V 147059-72-1
NTE STEREOSELECTIVE
REFERENCE COUNT: 2 TI

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

L9 ANSWER 4 OF 5
ACCESSION NUMBER:
TITLE:
131:116223 CASREACT
TITLE:
Process for preparing naphthyridones and intermediates
Chiu, Charles Krok-Pung, Wint, Lewin Theophilus
PATENT ASSIGNEE(S):
SOURCE:
COEN. EPXXDW

COEN. EPXXDW DOCUMENT TYPE: Patent English 2 LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: DATE PATENT NO. APPLICATION NO. DATE KIND 1 19990721 20030423 DE, DK, ES, V, FI, RO 1 19990805 2 19990921 1 20001121 20011128 20020421 20030515 EP 930297 EP 930297 A1 B1 EP 1999-300183 19990112 EP 930297 A1/
EP 930297 B1 R1 AT, EE, CH, D

IE, SI, LT, L

AU 9897115 A2

SG 76584 A1

EG 21514 A1

EG 21514 A1

EG 21514 B7

FF 930297 T

ES 2195513 T3

ER 9900066 A

CA 2258960 C

CA 2258960 C

CA 2258960 AA

NO 990185 A

EN 1228422 A

NZ 333769 A

AB G 64094 B1

PRIORITY APPIN. INFO::

GI GB, GR, IT, LI, LU, NL, SE, MC, PT, AU 1998-97115 19981215 AU 1998-97115 19981215
JP 1999-5494 19990112
SG 1999-46 19990112
TW 1999-88100415 19990112
AT 1999-300183 19990112
ES 1999-300183 19990112
ES 1999-66 19990114
CA 1999-2258960 19990114 20030515 20030829 20030829 20031201 20000509 20020903 19990716 19990719 19990915 20000327 20000717 NO 1999-185 CN 1999-101086 NZ 1999-333769 ZA 1999-277 19990115 19990115 19990115 BG 1999-103087 US 1998-71601P 20031231 MARPAT 131:116223

B 6-Acetamido-3-benzylazabicyclo[3.1.0]hexanes [I; Rl = (un)substituted PhCR2; R2 = Cl-6 alkyl, CF3, (un)substituted Ph] are prepared by reduction

the parent nitro derivs, with Fe powder in AcCH/Ne2CHUH and H-acylation of the resulting mines. Debenzylation of I with H in AccH in the presence of Pd catalyst, condensation of debenzylated intermediates with naphthyridine-3-carboxylate esters (II; R3 = C1-6 alkyl) and hydrolysis of

...G ===> U RX (5) OF 14

U: CM 2 YIELD 87%

RX(5) RCT G 232598-25-3
RGT I 75-75-2 MeSO3H
PRO U 147059-75-4
SOL 7732-119-5 Water, 71-36-3 BuOH
NTE extensive work-up to change crystal properties
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 5 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

129:122591 CASREACT

Diasterecoselective syntheses of N-protected derivatives of 1a, 5a, 6p-6-amino-3-azabicyclo[3.1.0] hexane. A route to trovafloxacin 6p-diasterecomer

AUTHOR(5):

AUTHOR(5):

Vilsmaier, Elmar; Goerz, Torsten
Fachbereich Chemie, Universitate Kaiserslautern,
Kaiserslautern, D-67663, Germany
Synthesis (1998), (5), 739-744
CODEN: SYNTEF; ISSN: 0039-7881

DOCUMENT TYPE:
LANGUAGE:

English

PUBLISHER: DOCUMENT TYPE: LANGUAGE: GI

N-protected derivs. of la,5a,6p-6-amino-3-azabicyclo[3.1.0]hexane (I) were synthesized via chloro enamines II (R = PhCH2, ally1). Specific N-protection was realized either by using a chloro enamine with different protecting groups or by selective removal of identical protecting groups at tribenzylated I. N.N'-dibenzylated I allowed the preparation of naphthyridine III.MeSO3M which represents the 6p-diasterecmer of trovafloxacin mesylate, a potent Gyrase inhibitor.

RX(14) OF 75 ...AP ---> AS

L9 ANSWER 4 OF 5 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

ANSWER 5 OF 5 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

AS: CM 2 YIELD 60%

RCT AP 210236-57-0 RGT AT 75-75-2 MeSO3H PRO AS 147126-01-0 SOL 7732-18-5 Water RX (14)

```
10/087,756
=> d his
     (FILE 'HOME' ENTERED AT 11:08:38 ON 18 APR 2005)
     FILE 'REGISTRY' ENTERED AT 11:08:42 ON 18 APR 2005
L1
               STRUCTURE UPLOADED
L2
              0 S L1SAM
L3
              0 S L1 SAM
              3 S L1 FULL
L4
     FILE 'CA' ENTERED AT 11:09:13 ON 18 APR 2005
L5
              3 S L4
     FILE 'CASREACT' ENTERED AT 11:10:22 ON 18 APR 2005
              0 S L1
L6
L7
              2 S L1 FULL
                STRUCTURE UPLOADED
L8
L9
              5 S L8 FULL
=>
---Logging off of STN---
```

Executing the logoff script...